

Mathematical Modeling Applied to Combustion Processes: Advances in the Theory of Combustion Modeling

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Introduction

Contextualization

Combustion modeling theory is an area of science that focuses on developing mathematical and computational models to describe and predict combustion processes, which occur when a fuel reacts with an oxidant, usually oxygen in the air. In this research, thermodynamic concepts, kinetic models and fluid mechanics models are applied to model an ideal combustion process in a combustion chamber of a jet engine in order predict the temperature variations in the combustor caused by the injection of hot gases into the chamber and by combustion.

Objectives

- Demonstrate the application of mathematical models based on physics and chemistry in combustion;
- Use mathematical models to describe the ideal combustion process in a combustion chamber of a reaction engine (jet engine).

Methodology

Extensive bibliography review and development of mathematical models.

Main Notation: T, Y_{fuel}, Y_{O_2} e $\dot{\omega}_i$

Preliminary Concepts: Combustion

General Combustion Equation: Combustion is a chemical reaction between a fuel and an oxidant, producing products, usually carbon dioxide CO_2 and water H_2O .

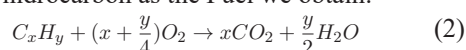
The general equation can be written as:



The fuels of interest include hydrocarbons C_xH_y such as:

- Gasoline $\approx C_8H_{15}$
- Kerosene $\approx C_{10}H_{22}$

Using a hydrocarbon as the Fuel we obtain:



Preliminary Concepts: Reaction Rate

Combustion can be *Lean*- excess oxidant, *Stoichiometric* - ideal amount of fuel and oxidant or *Rich*- excess fuel, depending on the *equivalence ratio*

$$\Phi = \frac{\left(\frac{m_{ox}}{m_{fu}}\right)_{est}}{\left(\frac{m_{ox}}{m_{fu}}\right)} \quad (3)$$

to be $\Phi < 1$, $\Phi = 1$ or $\Phi \geq 1$, respectively.

Reaction Rate (Law of Mass Action)

The fuel and oxygen consumption rates can be expressed as:

$$\dot{\omega}_{fuel} = \frac{d[C_xH_y]}{dt} = -k(T)[C_xH_y]^m[O_2]^n \quad (4a)$$

$$\dot{\omega}_{O_2} = \frac{d[O_2]}{dt} = -v_{O_2}'k(T)[C_xH_y]^m[O_2]^n \quad (4b)$$

Preliminary Concepts: Conservation Equations

The *reaction rate constant*, k , follows the Arrhenius model and varies with temperature according to:

$$k(T) = A \exp\left(\frac{-E_a}{R_u T}\right)$$

Where:

A = pre-exponential factor;
 E_a = activation energy;
 R_u = universal gas constant;
 T = absolute temperature.

Conservation Equations

These equations are fundamental for combustion modeling:

$$\text{Mass: } \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (5)$$

Preliminary Concepts: Heat Transfer

$$\text{Energy: } \rho c_p \left(\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T\right) = \nabla \cdot (k \nabla T) + Q \quad (6)$$

where Q is the *Heat Source* term due to chemical reactions:

$$Q = -\frac{\dot{\omega}_{fuel}}{M_{fuel}} \Delta H_{comb}$$

Species:
$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{v} Y_i) = \nabla \cdot (\rho D_i \nabla Y_i) + M_i \dot{\omega}_i \quad (7)$$

where Y_i represents the mass fraction of specie i .

Heat Transfer

Heat exchange with the surroundings follows Newton’s Law of Cooling that states

$$-k \frac{\partial T}{\partial n} = h [T_{surface} - T_{\infty}] \quad (8)$$

Preliminary Concepts: Numerical Method

Mass Flow Rate

The fuel and oxidant flow rate into the combustion chamber is modeled by

$$\left. \frac{\partial Y_i}{\partial x} \right|_{x=0} = -\frac{\dot{m}_i}{\rho u L_x} \quad (9)$$

Numerical Method: Finite Difference Method (FDM)

$$\frac{\partial \phi}{\partial t} = \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t}$$

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{1}{2} \left[\frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{(\Delta x)^2} + \frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{(\Delta x)^2} \right]$$

$$\frac{\partial \phi}{\partial x} = \frac{1}{2} \left[\frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} + \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} \right]$$

Combustion in Reaction Engines

Principle of Operation of a Reaction Engine (Jet Engine)

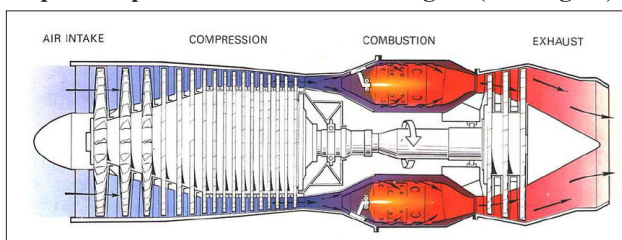


Figure: Principle of Operation of the Reaction Engine

Modeling. Numerical Approach

Mass Conservation inside the Chamber:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (10)$$

The Model. Numerical Approach

Equation solved by creating a velocity field $\mathbf{v} = (u, v)$ with

$u = u(x, y)$ e $v = v(x, y)$ that satisfies it:

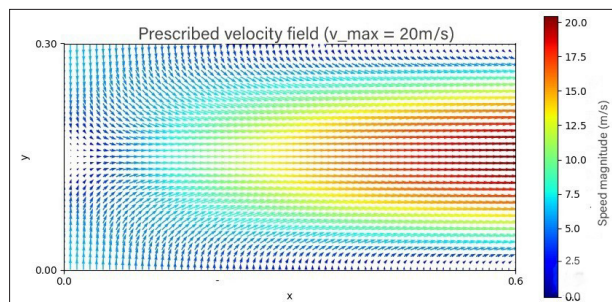


Figure: Prescribed Velocity Field

Thermal Energy Variation in the Chamber

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + \left(\frac{\Delta H_{comb}}{\rho c_p M_{fuel}} \right) \dot{\omega}_{fuel} \quad (11)$$

The Model. Numerical Approach

Ignition Model:

$$T(x, y, t = 0) = T_0 + \Delta T \cdot \exp \left[-\frac{(x - x_{ign})^2 + (y - y_{ign})^2}{\sigma^2} \right]$$

where $T_0 = 320K(47^\circ C)$ is the initial temperature in the chamber.

Applying the MDF to the energy equation, we obtain the system

$$\begin{aligned} -Smy_{i,j} T_{i+1,j}^{n+1} - Sby_{i,j} T_{i-1,i}^{n+1} + aT_{i,j}^{n+1} - Smx_{i,j} T_{i,j+1}^{n+1} - Sbx_{i,j} T_{i,j-1}^{n+1} = \\ Smy_{i,j} T_{i+1,j}^n + Sby_{i,j} T_{i-1,i}^n + bT_{i,j}^n + Smx_{i,j} T_{i,j+1}^n + Sbx_{i,j} T_{i,j-1}^n + q_{i,j} \end{aligned}$$

$$\Leftrightarrow \mathbf{A} \cdot \mathbf{T}^{n+1} = \mathbf{M} \cdot \mathbf{T}^n + \mathbf{Q}$$

$$\Leftrightarrow \mathbf{A} \cdot \mathbf{T}^{n+1} = \mathbf{B}$$

The Model. Numerical Approach

Variation of Chemical Species in the Chamber

Fuel: (11)

$$\frac{\partial Y_{fuel}}{\partial t} + u \frac{\partial Y_{fuel}}{\partial x} + v \frac{\partial Y_{fuel}}{\partial y} = D \left(\frac{\partial^2 Y_{fuel}}{\partial x^2} + \frac{\partial^2 Y_{fuel}}{\partial y^2} \right) + \frac{M_{fuel}}{\rho} \dot{\omega}_{fuel} \quad (12)$$

Oxygen:

$$\frac{\partial Y_{O_2}}{\partial t} + u \frac{\partial Y_{O_2}}{\partial x} + v \frac{\partial Y_{O_2}}{\partial y} = D \left(\frac{\partial^2 Y_{O_2}}{\partial x^2} + \frac{\partial^2 Y_{O_2}}{\partial y^2} \right) + \frac{M_{O_2}}{\rho} \left(\frac{m_{ar}}{m_{fu}} \right)_{est} \dot{\omega}_{fuel}$$

Similarly, applying the MDF, we obtain

$$\mathbf{A}_f \cdot \mathbf{Y}_f^{n+1} = \mathbf{M}_f \cdot \mathbf{Y}_f^n$$

$$\mathbf{A}_O \cdot \mathbf{Y}_O^{n+1} = \mathbf{M}_O \cdot \mathbf{Y}_O^n$$

Simulation Domain: Combustion Chamber

Ideal Combustion Chamber:

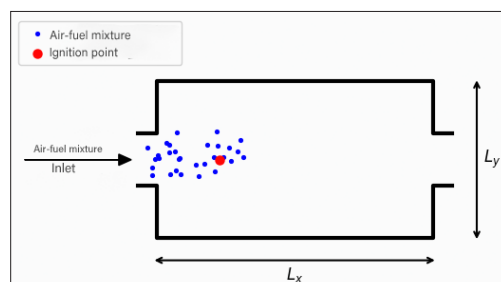
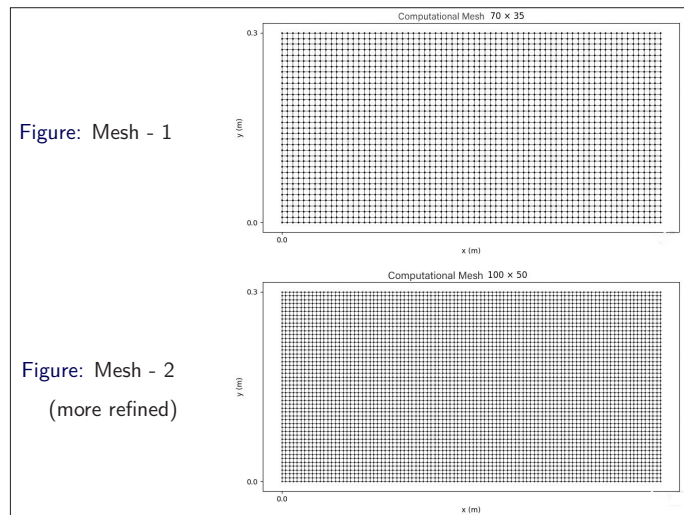


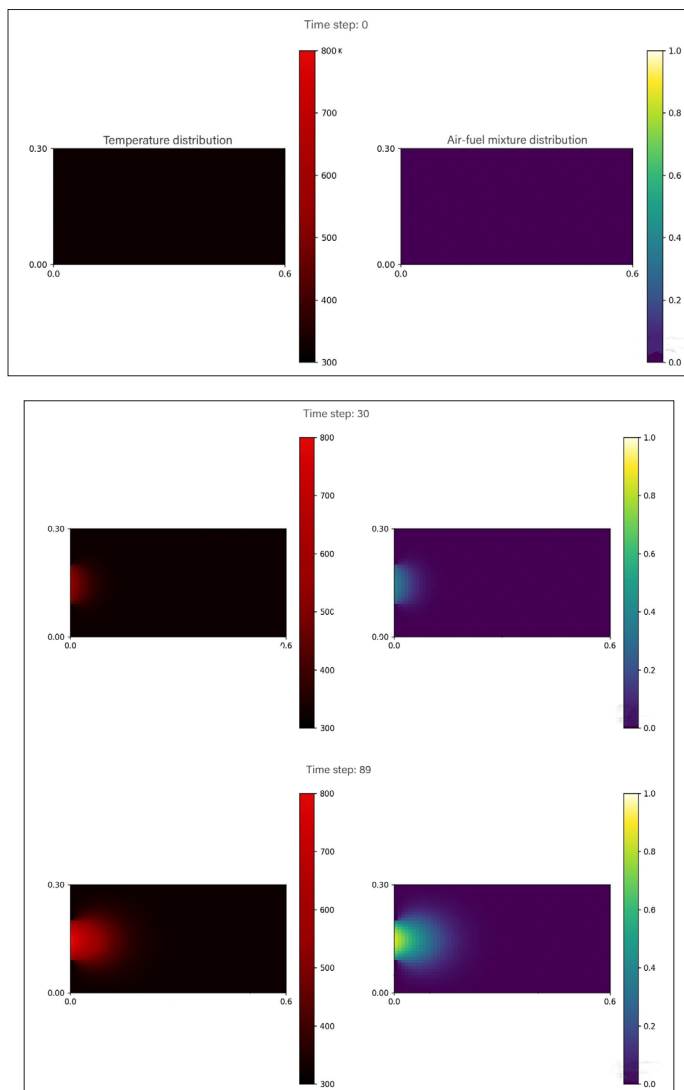
Figure: Ideal Combustion Chamber. Air and Fuel Inlet

Chamber Dimensions: $0, 6 \times 0, 3(m^2)$

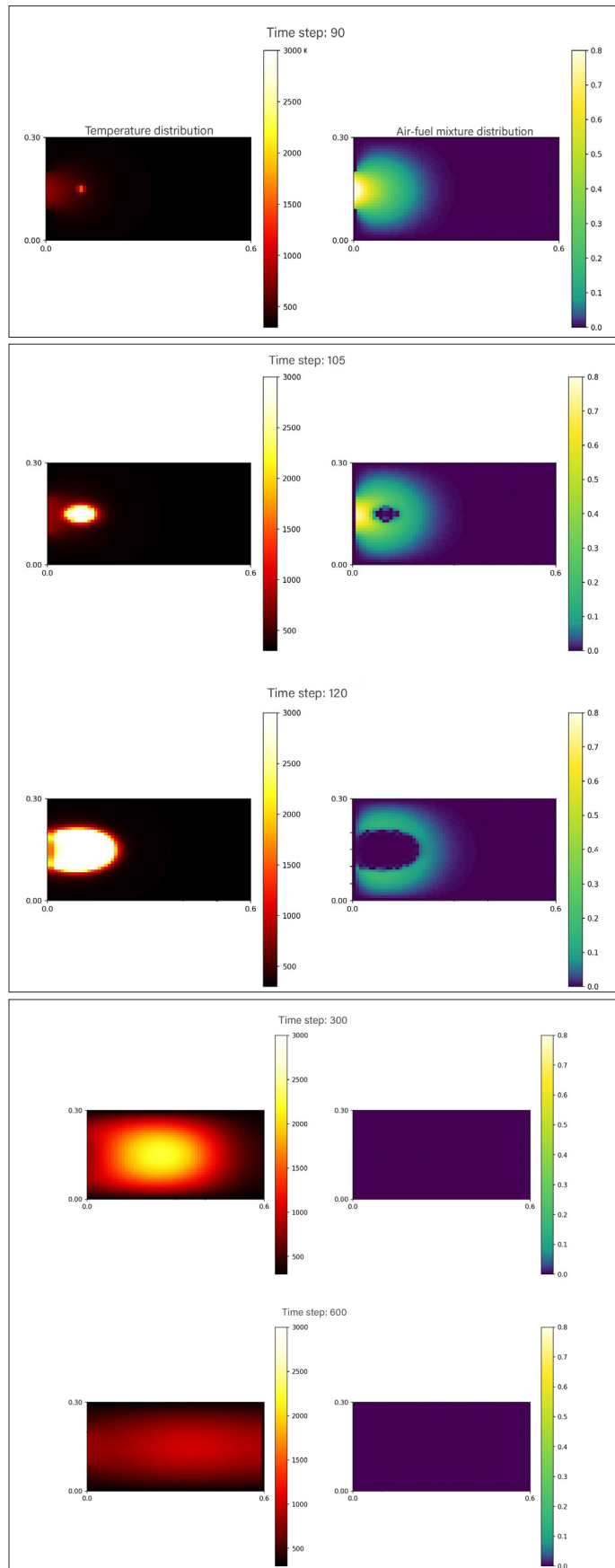
Simulation Domain: Numerical Meshes



**Results: Simulation 1 (Mesh - 1, $V = const$)
I: Injection of the Air-Fuel Mixture and Temperature Variation before Ignition:**

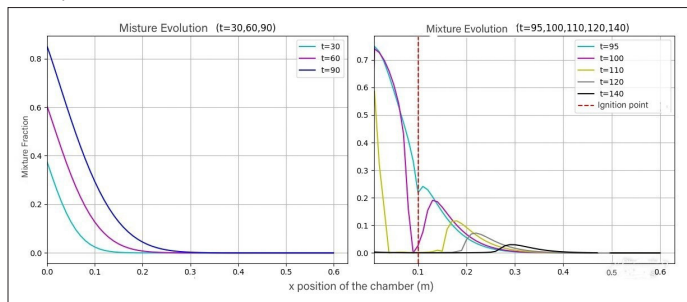


**Results: Simulation 1 (Mesh - 1, $V = const$)
II: Ignition, Air-Fuel Mixture Consumption, and Temperature Variation:**

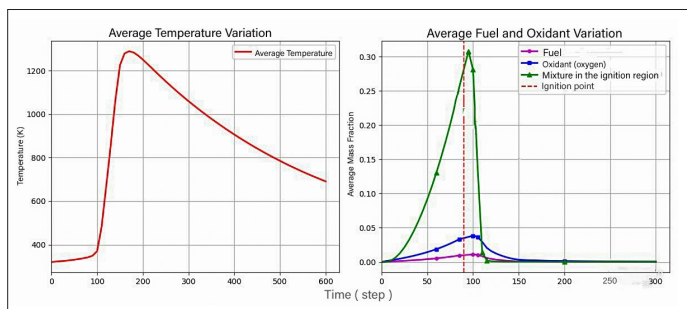


Results: Simulation 1 (Mesh1 - 1, $V = const$)

III: Variation of the Air-Fuel Mixture in the Combustor along $y = L_y/2$ before and After Ignition:

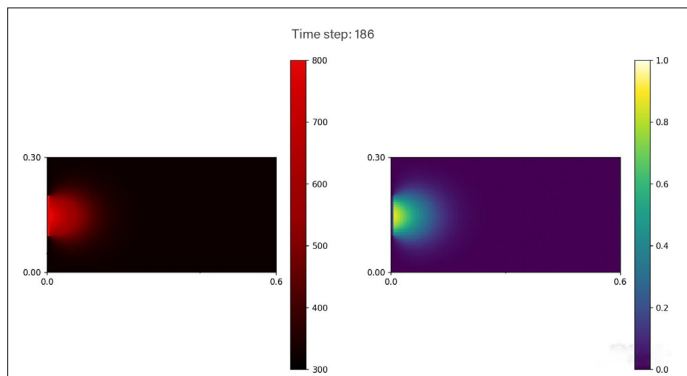


IV: Average Variation of Temperature, Oxidizer, and Fuel in the Combustor over Time:

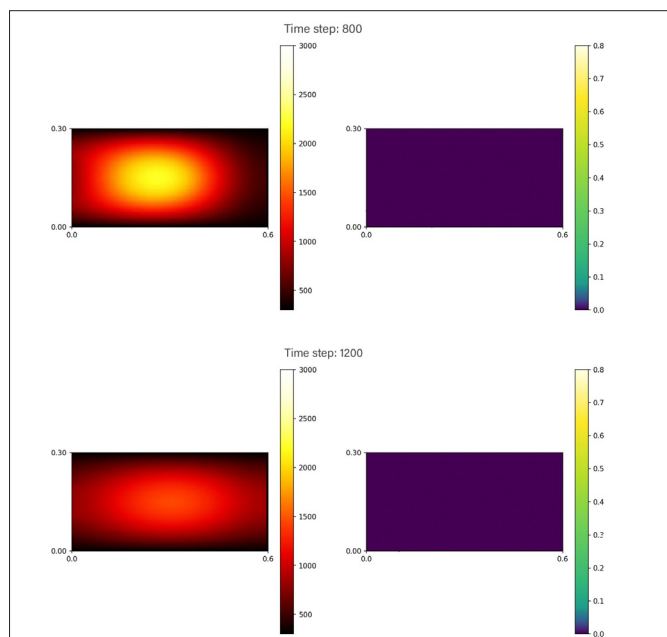
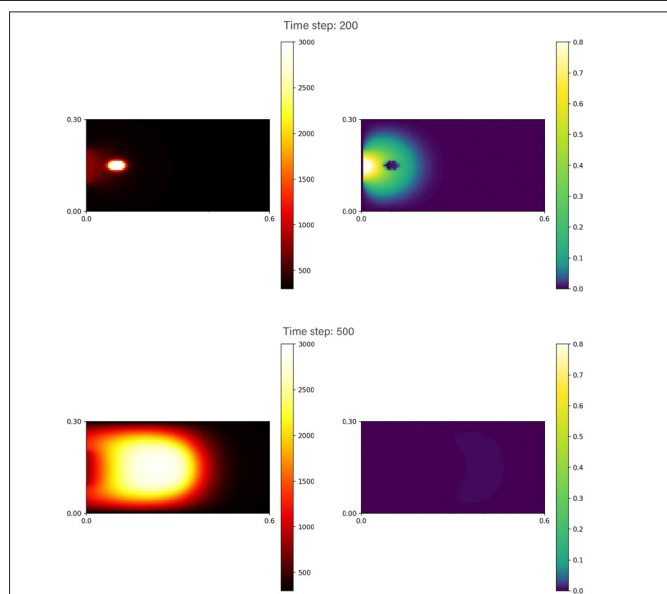
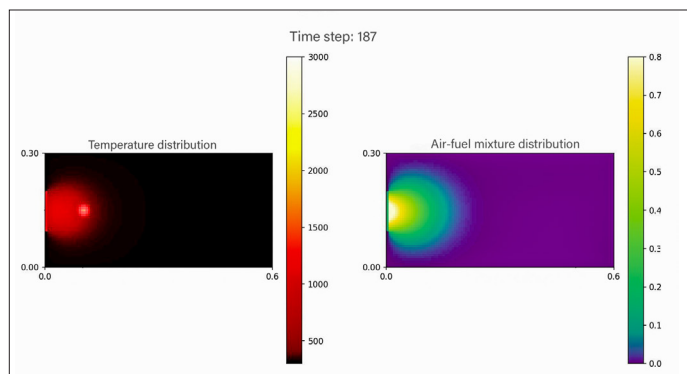


Results: Simulation 2 (Mesh - 2, $V = const$)

I: Injection of the Air-Fuel Mixture and Temperature Variation before Ignition:

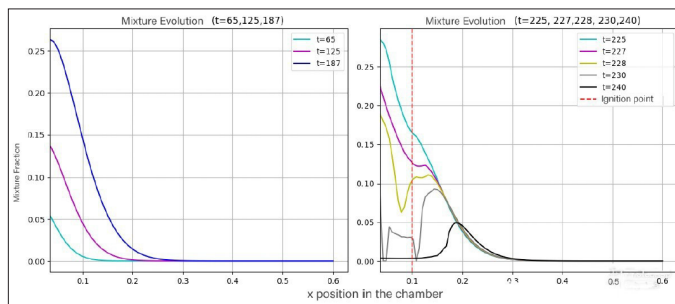


II. Ignition, Fuel-Air Mixture Consumption, and Temperature Variation:



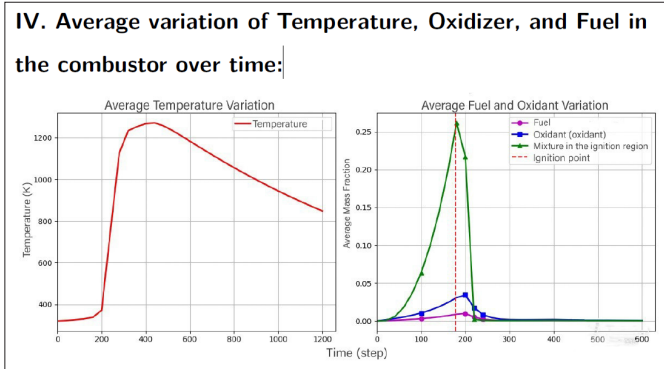
Results: Simulation 2 (Mesh - 2, $V = const$)

III: Variation of the Air-Fuel Mixture in the Combustor along $y = L_y/2$ before and after Ignition:



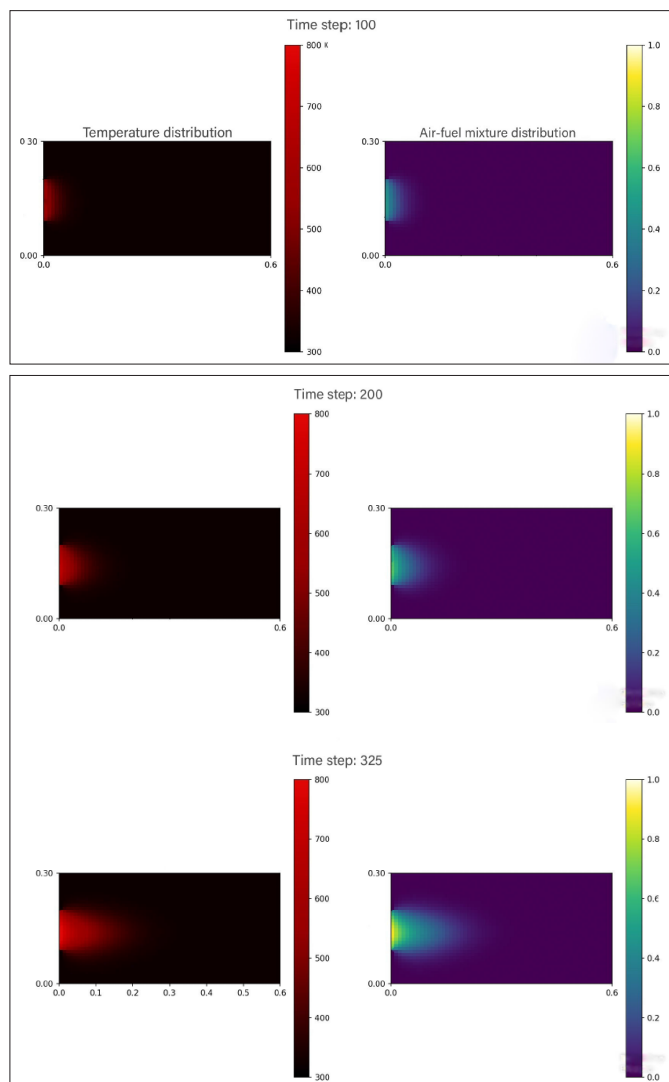
Results: Simulation 2 (Mesh - 2, $V = \text{const}$)

IV: Average Variation of Temperature, Oxidizer, and Fuel in the Combustor Over Time:



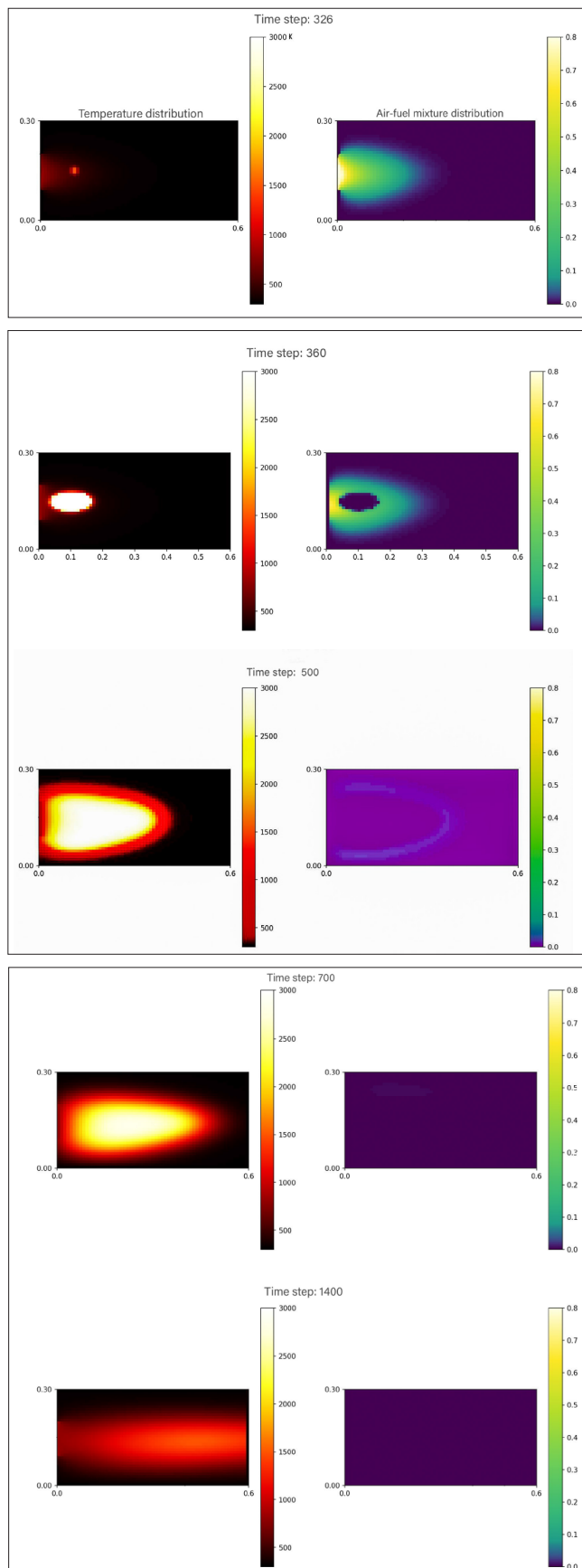
Results: Simulation 3 (Mesh - 1, $V = (u, v)(x, y)$)

I: Injection of the Air-Fuel Mixture and Variation of Temperature before Ignition:

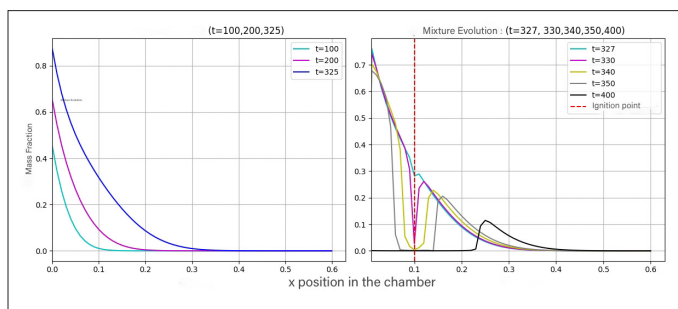


Results: Simulation 3 (Mesh - 1, $V = (u, v)(x, y)$)

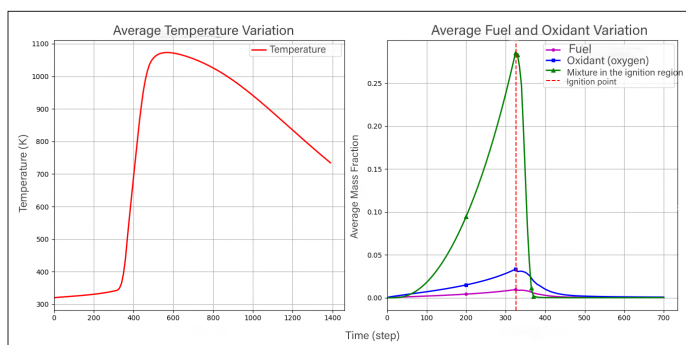
II: Injection of the Air-Fuel Mixture and Variation of Temperature before Ignition:



Results: Simulation 3 (Mesh - 1, $V = (u, v)(x,y)$)
III: Variation of the Air-Fuel Mixture in the Combustor along $y = L_y/2$ before and After Ignition:



IV: Average Variation of Temperature, Oxidizer, and Fuel in the combustor over time:



Conclusion

- Mathematical models serve as a bridge of connection between Problem—Solution in combustion field;
- The maximum temperature in the combustion chamber was around 3000K, which is about 500K higher than what has been predicted in combustion literature;
- The non-constant velocity field predicted results more aligned with the reality of combustion in jet engines according to the literature;
- There is a need to consider more detailed chemical mechanisms and refined physical parameters for more accurate results.

Future Work

- The computational cost of the Crank-Nicolson numerical method(version of the MDF used) is high. There is a need for more powerful computers to run the codes from more sophisticated models;
- There is a need to use more advanced numerical methods to simulate a chamber closer to the real one;
- There is a need for more powerful softwares (CFDs - ComputationalFluid Dynamics) for combustion studies. Python was used in this research.

References

1. Abreu AP (2023) Projeto de uma câmara de combustão anelar para um motor turbofan de pequenas dimensões. (Master thesis, Beira Interior University) [https://monografias.ufop.br/bitstream/35400000/3668/1/MONOGRRAFIA_Dimensio namentoC%C3%A2maraCombust%C3%A3o.pdf](https://monografias.ufop.br/bitstream/35400000/3668/1/MONOGRRAFIA_Dimensio%20namentoC%C3%A2maraCombust%C3%A3o.pdf).
2. Alves E (2024)The stationary combustion velocity in the presence of catalysts in the fuel composition. Method for calculating constants, Journal of Physical Mathematics and Its Applications, (London)
3. Alves E (2024)Overview of the current state of physical-mathematical modeling of solid fuel combustion processes,

Journal of Physical Mathematics and Its Applications, (London)

4. Alves E (2023) Exploring Theoretical Fundamentals of a Physical Mathematical Model for Unsteady Combustion in Solid Rocket Fuel and Developing Methods for Unsteady Velocity Calculation,Journal of Physical Mathematics and Its Applications, DOI: doi.org/10.47363/JPMA/2023 (London).
5. Atkins P, De Paula J (2006) Físico-Química. Livros Técnicos e Científicos, Editora S.A, (Rio de Janeiro).
6. Alves E (2018) Equation for calculating the burning rate of solid propellants. Far East Journal of Applied Mathematics 100: 153165.
7. Alves E (2007) Coecient calculation on the law speed of combustion of solid propellant, PermSTU Herald. Aerospace Engineering 4: 312.
8. Alves E (2000) Laws of combustion velocity of hard fuel containing catalysts, Proceedings of the Russian Scientific Technical Conference, PermSTU Herald. Aerospace Engineering, Perm, Russia 3: 38.
9. Alves E (2000) Mathematical model for non stationary process of combustion for hard fuel. The Second Polyakhov’s reading: Selected works. Saint-Petersburg State University, Saint-Petersburg, Russia 128-134.
10. Alves E (1999) Physic-mathematical model concretization of nonstationary combustion of solid propellant applied to problem of calculation of inside ballistic characteristics of missile motor. Perm STU Herald. Aerospace Engineering, Perm, Russia 3: 38.

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